Spatial Statistical Data Fusion for Remote Sensing Applications

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Outline

Definition

Data fusion is the process of combining information from heterogeneous sources into a single composite picture of the relevant process, such that the composite picture is generally more accurate and complete than that derived from any single source alone (Hall, 2004).

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Motivation: remote sensing data

What is the benefit of data fusion?

- Remote sensing data are often incomplete, sparse, and spatially and temporally heterogeneous. Our goal is to infer the true physical process from all available data sources.
- Data fusion capitalizes on complementary strengths of the individual datasets to minimize prediction errors.
- Correlation in *space* and *time* can be exploited for improved accuracy.

Estimating lower atmosphere CO2

- The lower atmosphere (below 500 hPa)is where CO_2 enters and exits the atmosphere. This may be a proxy for 'sources' and 'sinks'.
- No satellite instrument currently provides measurements of CO_2 globally near the Earth's surface.
- The Greenhouse gases Observing SATellite (GOSAT) provides total-column CO_2, while the Atmospheric InfraRed Sounder (AIRS) provides mid-tropospheric CO_2.
- Approximations to lower-atmospheric CO_2 may be made by deriving joint predictions of total-column CO_2 and mid-tropospheric CO_2 and taking a (weighted) difference.

Example of satellite orbits and footprints

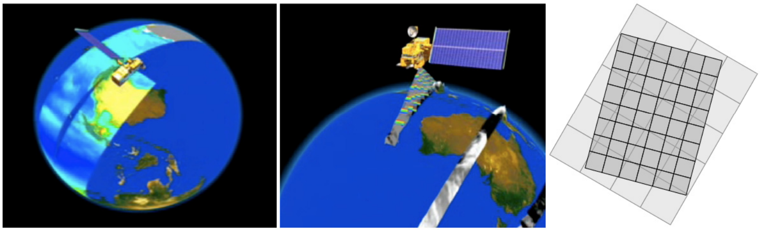

Figure: Example of different footprints (Source: Amy Braverman)

Difficulties of data fusion

Difficulties encountered when fusing remote sensing datasets:

- Massive size,
- Change of support,
- Isotropy and stationarity,
- Accounting for instruments' biases.

Outline

Introduction

Prelude: spatial (non-temporal) interpolation for massive datasets

Spatio-Temporal Data Fusion

Application to Lower Atmosphere CO2

Conclusion

Motivation

A special case of Spatio-Temporal Data Fusion is non-temporal spatial interpolation. It is convenient to introduce the ideas of STDF by talking about the spatial-only case first.

Data model

We assume the data from an instrument is generated according to the following model:

$$\begin{aligned} \mathbf{Z} &= (Z(B_1), Z(B_2), \ldots, Z(B_N))', \\ Z(B_j) &= \frac{1}{|D \cap B_j|} \left\{ \sum_{\mathbf{u} \in D \cap B_j} Y(\mathbf{u}) \right\} + \epsilon(B_j); \;\; B_j \subset \Re^d, \end{aligned}$$

where

- D is a discretized domain made up of Basic Areal Units (BAU),
- B_{ij} is the jth footprint from dataset $i (i = 1, 2)$,
- $\mathbf{Z}_i$ is the vector of response variable from dataset i,
- $Y(\cdot)$ is the true process,
- $\epsilon_i(B_{ij})$ is the error process.

Process model

We assume that the spatial process has the following linear mixed model (Cressie and Johannesson, 2008),

$$Y(\mathbf{s}) = \mathbf{t}(\mathbf{s})'\boldsymbol{\alpha} + \mathbf{S}(\mathbf{s})'\boldsymbol{\eta} + \xi(\mathbf{s}),$$

where

- $\xi(\cdot)$ is a fine-scale variation process (white noise) w/ variance σ_ξ^2,
- $\mathbf{t}(\mathbf{s})'\boldsymbol{\alpha}$ accounts for a linear trend,
- $\boldsymbol{\eta}$ is an r-dimensional Gaussian random vector $\mathrm{var}(\boldsymbol{\eta})$,
- $\mathbf{S}(\mathbf{s})$ is an r-dimensional spatial basis expansion of $\mathbf{s}$.

Covariance model

Given the linear mixed model, the covariance model is,

$$\mathbf{\Sigma} \quad \equiv \quad \mathrm{var}(\mathbf{Z}) = \mathbf{S}'\mathbf{K}\mathbf{S} + \sigma_\xi^2\mathbf{E} + \sigma_\epsilon^2\mathbf{V}.$$

where

- $\mathbf{K} = \mathrm{var}(\boldsymbol{\eta})$: fixed dimension $r \times r$,
- $\mathbf{S} \equiv (\mathbf{S}(B_1), \ldots, \mathbf{S}(B_N))'$,
- $\mathbf{E}$ and $\mathbf{V}$ are known matrices.

Prediction form

The optimal (linear unbiased) predictor of $Y(\mathbf{s})$ can be written as

$$\hat{Y}(\mathbf{s}) = \mathbf{a}'\mathbf{Z},$$

where $\mathbf{a}$ is an N-dimensional vector of kriging coefficients.

We wish to minimize,

$$\begin{aligned} E(Y(\mathbf{s}) - \hat{Y}(\mathbf{s}))^2 &= \mathrm{var}(Y(\mathbf{s}) - \mathbf{a}'\,\mathbf{Z}), \\ &= \mathrm{var}(Y(\mathbf{s})) - 2\mathbf{a}'\,\mathrm{cov}(\mathbf{Z}, Y(\mathbf{s})) + \mathbf{a}'\,\mathrm{var}(\mathbf{Z})\,\mathbf{a}, \end{aligned}$$

with respect to **a**, subject to the unbiasedness constraint,

$$\mathbf{0} = \mathbf{a}'\,\mathbf{T} - \mathbf{t}(\mathbf{s})'.$$

Solving using the method of Lagrange multipliers, the optimal kriging coefficients **a** is,

$$\mathbf{a}' = (\mathbf{c}' + (\mathbf{t}(\mathbf{s})' - \mathbf{c}'\,\boldsymbol{\Sigma}^{-1}\mathbf{T})(\mathbf{T}'\boldsymbol{\Sigma}^{-1}\mathbf{T})^{-1}\mathbf{T}')\,\boldsymbol{\Sigma}^{-1}.$$

Prediction and standard error equations

We can interpolate at a new location with the following,

$$\begin{aligned} Y(\mathbf{s})^{FRK} &= \mathbf{a}'\,\mathbf{Z}, \\ \sigma(\mathbf{s})^{SSDF} &= \left(\mathrm{E}(Y(\mathbf{s})^{SSDF} - Y(\mathbf{s}))^2\right)^{\frac{1}{2}} \\ &= \left(\mathbf{S}(\mathbf{s})'\mathbf{K}\mathbf{S}(\mathbf{s}) + \sigma_\xi^2 - 2\mathbf{a}'\left(\mathbf{S}'\mathbf{K}\mathbf{S}(\mathbf{s}) + \mathbf{b}(\mathbf{s})\right)\right. \\ &\quad \left. + \mathbf{a}'\left(\mathbf{S}'\mathbf{K}\mathbf{S} + \sigma_\xi^2\mathbf{E} + \mathbf{V}\right)\mathbf{a}\right)^{\frac{1}{2}}, \end{aligned}$$

where

$$\mathbf{b}(\mathbf{s}) = \mathrm{cov}(\boldsymbol{\xi}, \xi(\mathbf{s})).$$

This is called Fixed Rank Kriging.

Advantages of FRK

- Inversion of $\boldsymbol{\Sigma}$ is computationally scalable using the Sherman-Morrison-Woodbury formula (Hendersen and Searle, 1981),

$$\boldsymbol{\Sigma}^{-1} = \mathbf{U}^{-1} - \mathbf{U}^{-1}\mathbf{S}'\left(\mathbf{K}^{-1} + \mathbf{S}\mathbf{U}^{-1}\mathbf{S}'\right)^{-1}\mathbf{S}\mathbf{U}^{-1},$$

  where $\mathbf{U} = \sigma_{\xi}^{2}\mathbf{E} + \mathbf{V}$.
- No assumption of isotropy or stationarity.
- Handles change of support.
- Able to handle known systematic instrument biases.

Outline

Extending FRK to spatio-temporal data fusion

We develop an extension of FRK called Spatio-Temporal Data Fusion, which has the following properties,

- Ability to derive joint-estimates of two or more processes,
- Ability to exploit both spatial and temporal dependence in the data.

Main ideas behind STDF

- We account for temporal dependence using a first-oder auto-regressive model for $\boldsymbol{\eta}$.
- We do optimal predictions using a variant of the Kalman smoother.

Data model

We assume the data from an instrument is generated according to the following model:

$$Z_t^{(k)}(A) = \frac{1}{|D \cap A|} \left\{ \sum_{\mathbf{s} \in D \cap A} Y_t^{(k)}(\mathbf{s}) \right\} + \epsilon_t^{(k)}(A),$$

where

- $A \subset R^d$, $k = 1, 2$, $t = 1, 2, \ldots, T$,
- $Y_t^{(k)}(\cdot)$ is the true process,
- $\epsilon_t^{(k)}(A)$ is the error process.

Process model

We assume that the k-th process has the following form,

$$Y_t^{(k)}(\mathbf{s}) = \mathbf{x}_t^{(k)}(\mathbf{s})'\boldsymbol{\alpha}_t^{(k)} + \mathbf{S}_t^{(k)}(\mathbf{s})'\boldsymbol{\eta}_t^{(k)} + \xi_t^{(k)}(\mathbf{s}); \quad \mathbf{s} \in D.$$

where $\mathbf{x}_t^{(k)}(\cdot)$, $\boldsymbol{\alpha}_t^{(k)}$, $\mathbf{S}_t^{(k)}(\cdot)$, $\boldsymbol{\eta}_t^{(k)}$, and $\xi_t^{(k)}(\cdot)$ are defined in an analogous fashion to the corresponding spatial-only terms.

Instrument bias

To allow for bias, we assume that the measurement-error process may have non-zero mean,

$$\begin{aligned} \mathrm{E}(\epsilon_t^{(k)}(A)) &= c^{(k)}\mathrm{E}(Y^{(k)}(A)) \\ &= c^{(k)}\mathbf{x}(A)'\boldsymbol{\alpha}. \end{aligned}$$

- The multiplicative bias coefficients $\{c^{(k)} : k = 1, 2\}$ are assumed known.

Data stacking

At time t, we can stack datasets $\mathbf{Z}_t^{(1)}$ and $\mathbf{Z}_t^{(2)}$ to form a joint vector,

$$\begin{pmatrix} \mathbf{Z}_t^{(1)} \\ \mathbf{Z}_t^{(2)} \end{pmatrix} = \begin{pmatrix} \mathbf{X}_t^{(1)} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_t^{(2)} \end{pmatrix} \begin{pmatrix} \alpha_t^{(1)} \\ \alpha_t^{(2)} \end{pmatrix} + \begin{pmatrix} \mathbf{S}_t^{(1)} & \mathbf{0} \\ \mathbf{0} & \mathbf{S}_t^{(2)} \end{pmatrix} \begin{pmatrix} \eta_t^{(1)} \\ \eta_t^{(2)} \end{pmatrix} + \begin{pmatrix} \xi_t^{(1)} \\ \xi_t^{(2)} \end{pmatrix} + \begin{pmatrix} \epsilon_t^{(1)} \\ \epsilon_t^{(2)} \end{pmatrix},$$

or equivalently,

$$\mathbf{Z}_t = \mathbf{X}_t \alpha_t + \mathbf{S}_t \eta_t + \xi_t + \epsilon_t.$$

First-order auto-regressive temporal model

We assume that the covariance parameter $\boldsymbol{\eta}_t$ evolves according to a first-order auto regressive model,

$$\boldsymbol{\eta}_t | \boldsymbol{\eta}_{t-1}, \ldots, \boldsymbol{\eta}_0 \sim N_r\left(\mathbf{H}_t \boldsymbol{\eta}_{t-1}, \mathbf{U}_t\right); \; t = 1, 2, \ldots,$$

where

- The initial state is $\boldsymbol{\eta}_0 \sim N_r\left(\mathbf{0}, \mathbf{K}_0\right)$,
- The matrices $\mathbf{H}_t$ and $\mathbf{U}_t$ are called the propagator matrix and the innovation matrix.

Spatial-Temporal Data Fusion

Given data from two different instruments $\mathbf{Z}_1, \ldots, \mathbf{Z}_T$, we wish to optimally estimate the true processes at a set of locations $P \subset D$ at time $t \in \{1, \ldots, T\}$.

Assuming that the parameters $\boldsymbol{\alpha}$, $\mathbf{K}_0$, $\{(\sigma_\epsilon^{(k)})^2\}$, $\{(\sigma_\xi^{(k)})^2\}$, $\mathbf{H}_t$, and $\mathbf{U}_t$ are known, we can optimally estimate the posterior expectations and covariances for $\{\boldsymbol{\eta}_t\}$ and $\{\boldsymbol{\xi}_t^P\}$ using a variant of Kalman smoothing.

Kalman smoothing

Let $\mathbf{Z}_{1:\tilde{t}} \equiv (\mathbf{Z}'_1, \ldots, \mathbf{Z}'_{\tilde{t}})'$, we define,

- $\boldsymbol{\eta}_{t|\tilde{t}} \equiv \mathrm{E}(\boldsymbol{\eta}_t|\mathbf{Z}_{1:\tilde{t}})$,
- $\boldsymbol{\xi}^P_{t|\tilde{t}} \equiv \mathrm{E}(\boldsymbol{\xi}^P_t|\mathbf{Z}_{1:\tilde{t}})$,
- $\mathbf{P}_{t|\tilde{t}} \equiv \mathrm{var}(\boldsymbol{\eta}_t|\mathbf{Z}_{1:\tilde{t}})$,
- $\mathbf{R}^P_{t|\tilde{t}} \equiv \mathrm{var}(\boldsymbol{\xi}^P_t|\mathbf{Z}_{1:\tilde{t}})$,
- $\mathbf{W}^P_{t:\tilde{t}} \equiv \mathrm{cov}(\boldsymbol{\eta}_t, \boldsymbol{\xi}^P_t|\mathbf{Z}_{1:\tilde{t}})$.

Kalman smoothing

We first initialize $\boldsymbol{\eta}_{0|0} = \mathbf{0}$ and $\mathbf{P}_{0|0} = \mathbf{K}_0$. The one-step ahead forecasts are,

$$\begin{aligned} \boldsymbol{\eta}_{t|t-1} &= \mathbf{H}_t \boldsymbol{\eta}_{t-1|t-1} \\ \mathbf{P}_{t|t-1} &= \mathbf{H}_t \mathbf{P}_{t-1|t-1} \mathbf{H}'_{t|t}. \end{aligned}$$

The filtering quantities for $t = 1, \ldots, T$ are:

$$\begin{aligned}
\boldsymbol{\eta}_{t|t} &= \boldsymbol{\eta}_{t|t-1} + \mathbf{P}_{t|t-1}\mathbf{S}_t' \left[\mathbf{S}_t\mathbf{P}_{t|t-1}\mathbf{S}_t' + \mathbf{D}_t\right]^{-1}(\mathbf{Z}_t - \mathbf{Q}\mathbf{X}_t\boldsymbol{\alpha}_t - \mathbf{S}_t\boldsymbol{\eta}_{t|t-1}) \\
\boldsymbol{\xi}^P_{t|t} &= \mathbf{C}_t^{PZ}\mathbf{E}_t^{PZ} \left[\mathbf{S}_t\mathbf{P}_{t|t-1}\mathbf{S}_t' + \mathbf{D}_t\right]^{-1}(\mathbf{Z}_t - \mathbf{Q}\mathbf{X}_t\boldsymbol{\alpha}_t - \mathbf{S}_t\boldsymbol{\eta}_{t|t-1}) \\
\mathbf{P}_{t|t} &= \mathbf{P}_{t|t-1} - \mathbf{P}_{t|t-1}\mathbf{S}_t' \left[\mathbf{S}_t\mathbf{P}_{t|t-1}\mathbf{S}_t' + \mathbf{D}_t\right]^{-1}\mathbf{S}_t\mathbf{P}_{t|t-1} \\
\mathbf{R}^P_{t|t} &= \mathbf{C}_t^P\mathbf{E}_t^P - \mathbf{C}_t^{PZ}\mathbf{E}_t^{PZ} \left[\mathbf{S}_t\mathbf{P}_{t|t-1}\mathbf{S}_t' + \mathbf{D}_t\right]^{-1}(\mathbf{E}_t^{PZ})'(\mathbf{C}_t^{PZ})', \\
\mathbf{W}^P_{t|t} &= -\mathbf{P}_{t|t-1}\mathbf{S}_t' \left[\mathbf{S}_t\mathbf{P}_{t|t-1}\mathbf{S}_t' + \mathbf{D}_t\right]^{-1}(\mathbf{E}_t^{PZ})'(\mathbf{C}_t^{PZ})',
\end{aligned}$$

where $\mathrm{var}(\boldsymbol{\xi}_t^P) = \mathbf{C}_t^P\mathbf{E}_t^P$, $\mathrm{cov}(\boldsymbol{\xi}_t^P, \boldsymbol{\xi}_t) = \mathbf{C}_t^{PZ}\mathbf{E}_t^{PZ}$, and $\mathbf{Q}$ is a diagonal matrix with with $\{c^{(k)}\}$ along the diagonal.

Kalman smoothing

We obtain the smoothing quantities by updating "backwards" in time (i.e., for $t = T-1, T-2, \ldots, 0$):

$$\begin{aligned}
\boldsymbol{\eta}_{t|T} &= \boldsymbol{\eta}_{t|t} + \mathbf{J}_t(\boldsymbol{\eta}_{t+1|T} - \boldsymbol{\eta}_{t+1|t}) \\
\boldsymbol{\xi}^P_{t|T} &= \boldsymbol{\xi}^P_{t|t} + \mathbf{B}_t(\boldsymbol{\eta}_{t+1|T} - \boldsymbol{\eta}_{t+1|t}) \\
\mathbf{P}_{t|T} &= \mathbf{P}_{t|t} + \mathbf{J}_t(\mathbf{P}_{t+1|T} - \mathbf{P}_{t+1|t})\mathbf{J}'_t \\
\mathbf{R}^P_{t|T} &= \mathbf{R}^P_{t|t} + \mathbf{B}_t(\mathbf{P}_{t+1|T} - \mathbf{P}_{t+1|t})\mathbf{B}'_t, \\
\mathbf{W}^P_{t|T} &= \mathbf{W}^P_{t|t} + \mathbf{J}_t(\mathbf{P}_{t+1|T} - \mathbf{P}_{t+1|t})\mathbf{B}'_t,
\end{aligned}$$

where

$$\begin{aligned}
\mathbf{J}_t &\equiv \mathbf{P}_{t|t}\mathbf{H}'_{t+1}\mathbf{P}^{-1}_{t+1|t} \\
\mathbf{B}_t &\equiv -\mathbf{C}^{PZ}_t\mathbf{E}^{PZ}_t\left[\mathbf{S}_t\mathbf{P}_{t|t-1}\mathbf{S}'_t + \mathbf{D}_t\right]^{-1}\mathbf{S}_t\mathbf{P}_{t|t-1}\mathbf{H}'_{t+1}\mathbf{P}^{-1}_{t+1|t}.
\end{aligned}$$

Prediction equation

Having obtained the joint smoothing distribution of $\{\eta_t\}$ and $\{\xi_t^P\}$ given $\mathbf{Z}_1, \ldots, \mathbf{Z}_T$, the posterior mean of $\mathbf{Y}_t^P$ at the set of locations P at time t is,

$$\begin{aligned} \mathbf{Y}_{t|T}^P &= \begin{pmatrix} \mathbf{Y}_{t|T}^{(1)P} \\ \mathbf{Y}_{t|T}^{(2)P} \end{pmatrix} \\ &= \mathbf{X}_t^P \alpha_t + \mathbf{S}_t^P \eta_{t|T} + \xi_{t|T}^P. \end{aligned}$$

Prediction standard error matrix

The mean squared prediction error matrix (equivalently the posterior covariance matrix) can be calculated as:

$$\begin{aligned}
\mathbf{M}^{P}_{t|T} &\equiv \mathrm{E}\left(\left[\mathbf{Y}^{P}_{t} - \mathbf{Y}^{P}_{t|T}\right]\left[\mathbf{Y}^{P}_{t} - \mathbf{Y}^{P}_{t|T}\right]'\right) \\
&= \begin{pmatrix} \mathbf{M}^{(1,1)P}_{t|T} & \mathbf{M}^{(1,2)P}_{t|T} \\ \mathbf{M}^{(2,1)P}_{t|T} & \mathbf{M}^{(2,2)P}_{t|T} \end{pmatrix} \\
&= \mathbf{S}^{P}_{t}\mathbf{P}_{t|T}\mathbf{S}^{P'}_{t} + \mathbf{R}^{P}_{t|T} + 2\mathbf{S}^{P}_{t}\mathbf{W}^{P}_{t|T},
\end{aligned}$$

where $\mathbf{M}^{(k,m)P}_{t|T} \equiv \mathrm{E}\left(\left[\mathbf{Y}^{(k)P}_{t} - \mathbf{Y}^{(k)P}_{t|T}\right]\left[\mathbf{Y}^{(m)P}_{t} - \mathbf{Y}^{(m)P}_{t|T}\right]'\right)$.

Notes on STDF

STDF has attractive features that make it suitable for large remote sensing datasets,

- It is fast and scalable to large data inputs,
- It exploits the inter-process correlation for improved accuracy,
- It takes advantage of both *temporal* and *spatial* dependence in the data.

Outline

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Application to Lower Atmosphere CO2

Conclusion

Lower-atmosphere CO2

- Deriving global distribution of lower-atmosphere CO2 over time is important for studying 'sources' and 'sinks.'
- The Greenhouse gases Observing SATellite (GOSAT) provides total-column CO_2, while the Atmospheric InfraRed Sounder (AIRS) provides mid-tropospheric CO_2.
- We will derive joint predictions of total-column CO_2 and mid-tropospheric CO_2 and taking a (weighted) difference to obtain lower atmosphere CO2.

Application outline

- We select GOSAT and AIRS data over the continental United States between June and August of 2009.
- We make joint-prediction of total-column CO2 and mid-tropospheric CO2, and use weighted differencing to derive predictions of lower atmosphere CO2.
- Predictions of lower atmosphere CO2 will be compared to coincident aircraft data from NOAA.
- We also compare the performance of STDF with an alternative interpolation methodology (locally weighted regression).

Observing tracks and atmospheric sensitivity

Example of satellite orbits and sensitivity

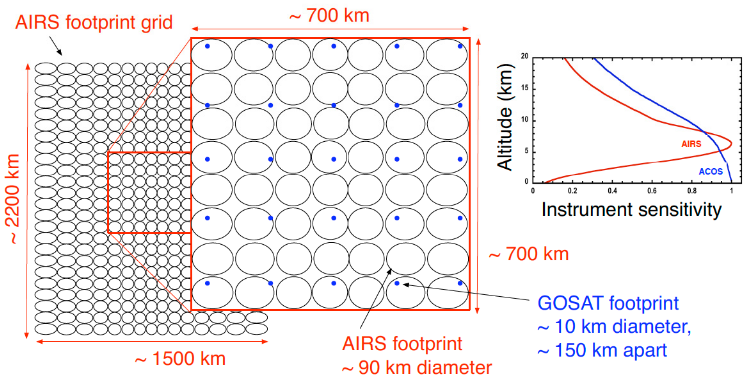


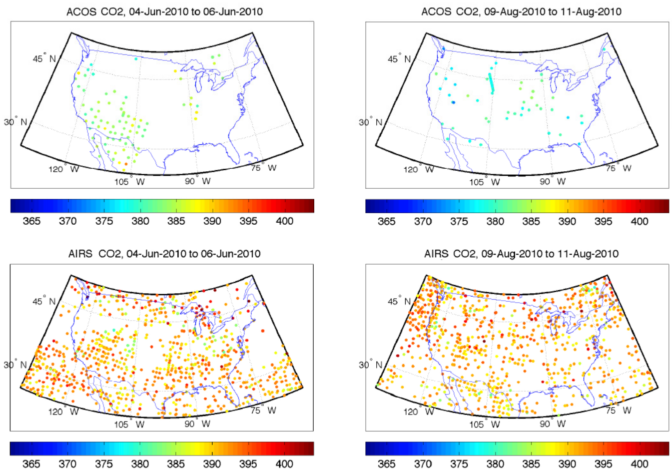
Figure: Example of GOSAT and AIRS sensitivity

ACOS and AIRS input data

- Within our domain, we have 3,869 ACOS data points and 40,564 AIRS data points.
- We group the data over these three months into 3-day blocks.
- For the elements of the vector of basis functions, we use local bisquare functions.
- The covariate function $\mathbf{t}(\cdot)$ are defined using a constant 1, latitude, and longitude.
- Given the joint prediction, $(\hat{Y}_{t|T,ACOS}(\mathbf{s}), \hat{Y}_{t|T,AIRS}(\mathbf{s}))'$, we estimate lower atmosphere CO2 as a simple linear combination

$$\hat{Y}_{t|T,LA}(\mathbf{s}) = \frac{7}{5}\hat{Y}_{t|T,ACOS}(\mathbf{s}) + \frac{2}{5}\hat{Y}_{t|T,AIRS}(\mathbf{s}).$$

Example of input data



STDF output example

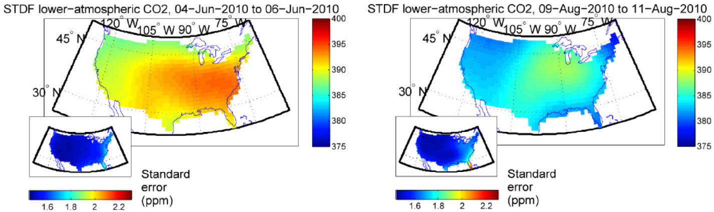


Figure: STDF output

- Run time for entire 3-month period: 4 minutes on a 3.06 GHz machine with an Intel Duo Core processor.

NOAA lower-atmosphere CO2 data

- The National Oceanic and Atmospheric Administration (NOAA) has been sampling lower-atmospheric CO_2 through a series of aircraft flights over Beaver Crossing, Nebraska and Lamont, Oklahoma.
- We can compare the NOAA aircraft data at these two locations against the corresponding 95% confidence intervals for STDF lower-atmospheric CO_2.

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NOAA lower-atmosphere CO2 comparison

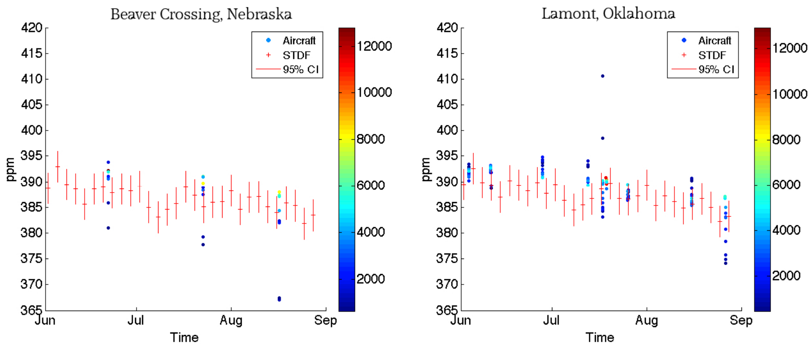
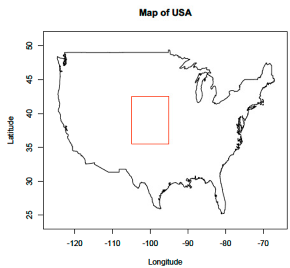


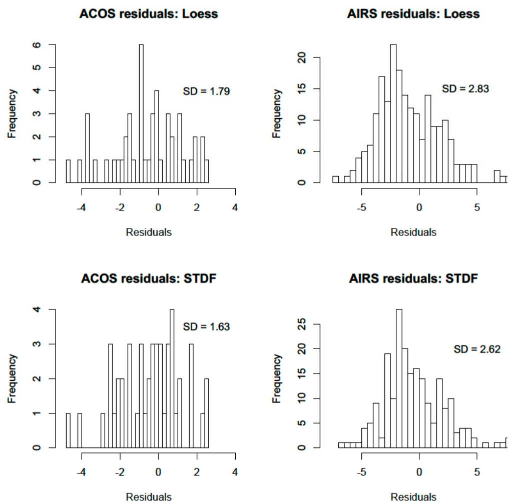
Figure: STDF outputs (red intervals) vs NOAA data (colored circles).

Comparison vs loess

- To compare against loess, we randomly 6 time blocks, and designate a small, fixed area as a reserve region.
- All data falling within the reserve region within those 6 time blocks are withheld as test data.
- We apply STDF and loess predict the value of ACOS and AIRS CO2 at the test locations.



Comparison vs loess - results



Outline

Conclusions

- STDF is fast: feasible for large remote sensing datasets.
- Results look reasonable by comparison to aircraft data for this example.
- Applicable to other types of remote sensing data, e.g., aerosols, clouds, soil moisture...
- Extensions: Bayesian inference, application to remote sensing radiances, etc.
- Questions and/or comments: contact Hai Nguyen at hai.nguyen@jpl.nasa.gov.

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Appendix

EM estimation

Let $\boldsymbol{\theta}^{[b]}$ be the parameter vector at the b-th EM iteration. The conditional expectations and covariance matrices for the "missing data" are defined as:

$$
\begin{aligned}
\boldsymbol{\eta}_{t|T}^{[b]} &\equiv \mathrm{E}_{\boldsymbol{\theta}^{[b]}}(\boldsymbol{\eta}_t|\mathbf{Z}_{1:T}) \\
\boldsymbol{\xi}_{t|T}^{[b]} &\equiv \mathrm{E}_{\boldsymbol{\xi}^{[b]}}(\boldsymbol{\xi}_t|\mathbf{Z}_{1:T}) \\
\mathbf{P}_{t|T}^{[b]} &\equiv \mathrm{var}_{\boldsymbol{\theta}^{[b]}}(\boldsymbol{\eta}_t|\mathbf{Z}_{1:T}) \\
\mathbf{R}_{t|T}^{[b]} &\equiv \mathrm{var}_{\boldsymbol{\theta}^{[b]}}(\boldsymbol{\xi}_t|\mathbf{Z}_{1:T}) \\
\mathbf{W}_{t|T}^{[b]} &\equiv \mathrm{cov}_{\boldsymbol{\theta}^{[b]}}(\boldsymbol{\eta}_t,\boldsymbol{\xi}_t|\mathbf{Z}_{1:T}) \\
\mathbf{P}_{t,t-1|T}^{[b]} &\equiv \mathrm{cov}_{\boldsymbol{\theta}^{[b]}}(\boldsymbol{\eta}_t,\boldsymbol{\eta}_{t-1}|\mathbf{Z}_{1:T}).
\end{aligned}
$$

The cross-covariance term, $\mathbf{P}_{t,t-1|T} \equiv \mathrm{cov}(\boldsymbol{\eta}_t, \boldsymbol{\eta}_{t-1}|\mathbf{Z}_{1:T})$, is given by,

$$\begin{aligned}
\mathbf{P}_{T,T-1|T} &= (\mathbf{I}_r - \mathbf{P}_{T|T-1}\mathbf{S}'_T\left[\mathbf{S}_T\mathbf{P}_{T|T-1}\mathbf{S}'_T + \mathbf{D}_T\right]^{-1}\mathbf{S}_T) \\
&\quad \times \mathbf{H}_T\mathbf{P}_{T-1|T-1} \\
\mathbf{P}_{t,t-1|T} &= \mathbf{P}_{t|t}\mathbf{J}'_{t-1} + \mathbf{J}_t(\mathbf{P}_{t+1,t|T} - \mathbf{H}_{t+1}\mathbf{P}_{t|t})\mathbf{J}'_{t-1},
\end{aligned}$$

where $\mathbf{I}_r$ is the $r \times r$ identity matrix, and define,

$$\mathbf{L}_t^{[b+1]} \equiv \mathbf{P}_{t,t-1|T}^{[b]} + \boldsymbol{\eta}_{t|T}^{[b]}\boldsymbol{\eta}_{t-1|T}^{[b]\prime}.$$

EM estimation

The EM updates for $\boldsymbol{\theta}^{[b+1]}$ are:

$$\begin{aligned}
\alpha_t^{[b+1]} &= (\mathbf{X}_t'\mathbf{Q}\mathbf{V}_t^{-1}\mathbf{Q}\mathbf{X}_t)^{-1}\mathbf{X}_t'\mathbf{Q}\mathbf{V}_t^{-1}\left[\mathbf{Z}_t - \mathbf{S}_t\eta_{t|T}^{[b]} - \xi_{t|T}^{[b]}\right], \\
\mathbf{K}_0^{[b+1]} &= \mathbf{P}_{0|T}^{[b]} + \eta_{0|T}^{[b]}\eta_{0|T}^{[b]\prime} \\
(\sigma_{\xi,t}^{(1)})^{2\ [b+1]} &= \frac{1}{N_t^{(1)}}\text{trace}\left(\left(\mathbf{E}_t^{-1}\left[\mathbf{R}_{t|T}^{[b]} + \xi_{t|T}^{[b]}\xi_{t|T}^{[b]\prime}\right]\right)_{[1,N^{(1)}]}\right) \\
(\sigma_{\xi,t}^{(2)})^{2\ [b+1]} &= \frac{1}{N_t^{(2)}}\text{trace}\left(\left(\mathbf{E}_t^{-1}\left[\mathbf{R}_{t|T}^{[b]} + \xi_{t|T}^{[b]}\xi_{t|T}^{[b]\prime}\right]\right)_{[N^{(1)}+1,N]}\right) \\
\mathbf{H}^{[b+1]} &= \left(\sum_{t=1}^{T}\mathbf{L}_t^{[b+1]}\right)\left(\sum_{t=0}^{T-1}\mathbf{K}_t^{[b+1]}\right)^{-1} \\
\mathbf{U}^{[b+1]} &= \left(\sum_{t=1}^{T}\mathbf{K}_t^{[b+1]} - \mathbf{H}^{[b+1]}\sum_{t=1}^{T}\mathbf{L}_t^{[b+1]\prime}\right)/T.
\end{aligned}$$

EM estimation

Convergence of the parameter estimates may be monitored through the negative log-likelihood

$$-\log L(\boldsymbol{\theta}) = \frac{1}{2}\sum_{t=1}^{T} \log |\boldsymbol{\Sigma}_{\beta,t}(\boldsymbol{\theta})| + \frac{1}{2}\sum_{t=1}^{T} \boldsymbol{\beta}_t' \boldsymbol{\Sigma}_{\beta,t}(\boldsymbol{\theta})^{-1} \boldsymbol{\beta}_t .$$

Weighted differencing

We make the following simplifying assumptions,

- The air pressure at the surface of the Earth is 1000 hectopascals (hPa) and the air pressure at the satellite instrument is 0 hPa.
- The middle troposphere is the portion of the atmosphere between 500 hPa and 300 hPa.
- The CO_2 concentration above 300 hPa can be ignored.

Weighted differencing

Given total column CO_2, $Y_{\mathrm{ACOS}}(\mathbf{s})$, and mid-tropospheric CO_2, $Y_{\mathrm{AIRS}}(\mathbf{s})$, at a location $\mathbf{s}$, we approximated lower-atmospheric CO_2, $Y_{\mathrm{LA}}(\mathbf{s})$, as a simple linear combination,

$$\begin{aligned} Y_{\mathrm{LA}}(\mathbf{s}) &= \frac{(1000-300)\,Y_{\mathrm{ACOS}}(\mathbf{s}) - (500-300)\,Y_{\mathrm{AIRS}}(\mathbf{s})}{1000-500} \\ &= \frac{7}{5}Y_{\mathrm{ACOS}}(\mathbf{s}) - \frac{2}{5}Y_{\mathrm{AIRS}}(\mathbf{s}). \end{aligned}$$

Weighted differencing

From the weighted difference above, it is straightforward to obtain the prediction standard error at location **s**,

$$\sigma^2_{\mathrm{LA}}(\mathbf{s}) \equiv \left(\; 7/5, -2/5 \; \right) \mathbf{M}_{t|T}(\mathbf{s}) \left(\; 7/5, -2/5 \; \right)',$$

where $\mathbf{M}_{t|T}(\mathbf{s})$ is the prediction-error matrix for the $\mathrm{CO_2}$ prediction vector $\hat{Y}_{t|T}(\mathbf{s}) \equiv (\hat{Y}_{t|T,ACOS}(\mathbf{s}), \hat{Y}_{t|T,AIRS}(\mathbf{s}))'$.